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Eigenvalue Problems without Detailed Balance Condition

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The second largest eigenvalue of transition rate matrix in Markov chain without detailed balance condition is investigated. Recent studies on Markov chain Monte Carlo method have found that the convergence to equilibrium distribution speeds up under the violation of detailed balance condition [1-4]. However, mathematical proof for such acceleration of the convergence has not been given. Since the typical time of convergence is governed by the second largest eigenvalue of the transition matrix, which characterizes the Markov chain, the violation of the detailed balance condition is expected to relate with decrease of the second largest eigenvalue. We prove that the second largest eigenvalue always decreases introducing the violation of detailed balance condition.

We consider the irreducible Markov process over N discrete states

$$\frac{dP_i(t)}{dt} = \sum_{j=1}^{N} q_{ij} P_j(t) - \sum_{j=1}^{N} q_{ji} P_i(t), \tag{1}$$

where $P_i(t)$ is the probability of the microstate i at time t, q_{ij} denotes the transition rate from state j to state i. This equation is rewritten as

$$\frac{dR_i(t)}{dt} = \sum_{j(\neq i)} w_{ij} R_j(t) - \sum_{j(\neq i)} q_{ji} R_i(t) = \sum_{j=1}^{N} W_{ij} R_j(t) \tag{2}$$

by introducing the variables $R_i(t) = P_i(t)/\sqrt{\pi_i}$, $W_{ij} = w_{ij} = \pi_i^{-1/2} q_{ij} \pi_j^{1/2}$ for $i \neq j$, $W_{ii} = -\sum_{j(\neq i)} q_{ji}$ with the target probability π_i. In this form, the detailed balance condition is represented by the symmetry of W_{ij}. Then we decompose W into its symmetric and anti-symmetric parts. The systematic proof of the acceleration of the convergence by the violation of the detailed balance condition is then given from the perspective of the effect of the modulation in the symmetry of W on the eigenvalues. The proof employs Ostrowski-Taussky inequality [5], which describes the relation between eigenvalues of the transition matrices with and without detailed balance condition.

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